

# Probability Density Function Characterization for Conditional Source-term Estimation in High-Pressure Combustion

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The present study investigates the long-standing issue in the accurate simulations of high-pressure (high- $p$ ) combustion, namely: the modeling of turbulence-chemistry - thermodynamic interaction. This issue is addressed through an a posteriori study of a Direct Numerical Simulation (DNS) database representing high- $p$  turbulent combustion. The DNS database is described in Bellan (2017) and consists of simulations of a temporal mixing layer in which a single-step chemical reaction occurs. That study indicates that when the single-conditioned Conditional Source-term Estimate (CSE) approach is used based on a beta probability distribution function (PDF) representing the mixture fraction, the turbulent reaction rate is significantly over-predicted; the inaccuracy of the model is here traced to the large variance about the conditional mean due to the non-linearity in the real-gas equation of state. It is shown that by doubly-conditioning the source-term using as conditioning variables the mixture fraction and a characteristic thermodynamic variable, the chemical source-term estimation is considerably improved for all test cases in the DNS database. The rationale directing the choice of the PDF and the reason for the Double-Conditioned Source-term Estimate approach success are explained.

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## 1. Introduction

One of the most challenging issues in modeling, simulating and accurately predicting turbulent combustion is the accurate modeling of the turbulent reaction rate. Whereas substantial progress has been made over the last decade in this area for atmospheric- $p$  combustion [1], and most generally for situations obeying perfect-gas physics, there has been a lack of success in modeling this rate for high- $p$  combustion. The situation is particularly concerning given the fact that virtually all engines used in transportation –e.g. diesel and gas turbine engines– and in propulsion – e.g. liquid-rocket engine – rely on high- $p$  combustion in which the high- $p$  feature is used to accelerate the chemical reactions and increase heat release.

The physical complexity of high- $p$  combustion imposes stringent demands on predictive simulations. Indeed, at these high- $p$  conditions, the non-negligible intermolecular

forces – and the resulting thermodynamics and transport properties – present additional challenges for predictive combustion simulations. At these extreme conditions, a real-fluid equation of state (EOS) must be used in conjunction with appropriate mixing rules. Additionally, for the multi-species situations encountered in combustion, a fully-populated diffusion matrix is needed to account for the physics of the problem. In most engineering-relevant cases, the resolution of all these concurrent physical processes on the appropriate time and spatial scale remains computationally intractable. For this reason, most modeling approaches must rely on a method to limit the range of scales requiring resolution. In one of the most promising approaches, Large Eddy Simulation (LES), the conservation equations are filtered to remove the small scales and models are used in these conservation equations to mimic the behavior of these unresolved small scales. Because the unresolved scales play a particularly important role in combustion by mixing at scales of the order of the Kolmogorov scales, thus capturing the output of the molecular mixing, the turbulent reaction rate is substantially driven by the small-scale turbulent fluctuations. Bellan [2] showed that several of the assumptions pivotal to perfect-gas turbulence-chemistry interaction models are not satisfied for high- $p$  combustion.

The generic difficulty with modeling the turbulent reaction rate is inherently due to the non-linear Arrhenius expression through which the reaction rate depends on the thermodynamic variables. Thus, even a small change in the temperature  $T$ , density  $\rho$  or species mass fraction  $Y_\alpha$  where  $\alpha$  refers to the species, will lead to large variations in the value of the turbulent reaction rate [3]. For high- $p$  reactive flows the reaction rate non-linearity is compounded by the strong non-linearity of the EOS thus leading to the necessity to account for *turbulent-chemistry-thermodynamic interactions* when modeling the turbulent reaction rate.

When considering LES, and denoting a filtered quantity by  $\overline{(\cdot)}$ , the above discussion leads to the conclusion that

$$\overline{\dot{\omega}}(\rho, T, Y_\alpha) \neq \dot{\omega}(\bar{\rho}, \bar{T}, \bar{Y}_\alpha) \quad (1.1)$$

where  $\dot{\omega}$  represents the reaction rate. The inequality also holds true for averaged quantities (denoted here as  $\langle \cdot \rangle$ ). The modeling philosophy for mitigating the problem introduced by Eq. (1.1) is to introduce a mapping technique so as in the new frame, the filtered reaction rate has a smaller variation than in the physical space, with the hope that this constrained variation will lend to easier modeling; if so, a reverse mapping could produce  $\overline{\dot{\omega}}$  in the physical space. For perfect-gas reactive flow, this mapping was achieved by Steiner and Bushe [3] by conditionally averaging  $\dot{\omega}$  and the approach was labeled the Conditional Source-term Estimation (CSE) method; the word “Source” refers to the fact that  $\overline{\dot{\omega}}$  is a source in the conservation equation for the species. In the CSE method, the pivotal ingredients to success are the judicious selection of the dependent variable on which  $\overline{\dot{\omega}}$  is conditioned and the accuracy of the probability density function (PDF) of this variable. More recently, it has been shown that by choosing two such dependent variables rather than one, the success of the method is increased [15]; this modified method has been referred to as the Doubly Conditional Source-term Estimation (DCSE) method. The increased success of DCSE with respect to CSE stems from the fact that additional conditioning leads to decreasing the variance with respect to the dependent variables used for conditioning, and thus restricts the region in which the model must be constructed, potentially leading to a higher-fidelity model.

This study is devoted to investigating the probability density function for high- $p$  reac-

tive flows by comparing the estimated source-term computation with a Direct Numerical Simulation (DNS) database of high- $p$  five-species mixing and single-step reaction. Both issues of the correct representation of the PDF and of the number of conditioning variables will be addressed. In particular, the applicability of the well-established atmospheric- $p$  PDF models to high- $p$  combustion will be explored. In this report we first summarize the CSE model in 2, and then we describe the DNS database in 4. In the results section 4 we first study the applicability of CSE using atmospheric- $p$  to high- $p$  combustion and address the form of the PDF as well as the influence of the mixture fraction definition. The limited success obtained with CSE prompted the evaluation of a DCSE model using  $T$ , as a major thermodynamic variable of interest, for the further conditioning. The accurate source term estimate thus obtained, even by using a PDF which lacked in accuracy, is explained. A summary and conclusions follow in section 4.

## 2. Brief Description of the Conditional Source-term Estimation Method

The CSE method was developed by Bushe and Steiner [12] as a computationally advantageous extension of the Conditional Moment Closure. Both approaches stem from the observation that the fluctuations of the reactive species and the mixture fraction are correlated; thus, when conditioned on the mixture fraction, the dependent variables have a smaller variation about the conditional mean than in physical space. The central tenet of CSE is that

$$\overline{\dot{\omega}}|\zeta \approx \dot{\omega} \left( \overline{\rho}|\zeta, \overline{T}|\zeta, \overline{Y_\alpha}|\zeta \right), \quad (2.1)$$

where  $\zeta$  is the conditioning variable taken here as the mixture fraction. If the PDF of  $\zeta$ ,  $P(\zeta)$ , is known, then one can obtain estimates of the conditioned thermodynamic quantities meaning that one can map the spatial variation of each dependent variable to a variation of that dependent variable in the vicinity of  $P(\zeta)$ . The reverse mapping is

$$\overline{\dot{\omega}}_{CSE} = \int_0^1 P(\zeta) \overline{\dot{\omega}}|\zeta d\zeta \approx \int_0^1 P(\zeta) \dot{\omega} \left( \overline{\rho}|\zeta, \overline{T}|\zeta, \overline{Y_\alpha}|\zeta \right) d\zeta, \quad (2.2)$$

showing the crucial role of the accurate knowledge of  $P(\zeta)$  in achieving success. From this formulation, it is clear that the closure of the mean chemical source term highly depends on the accurate representation of the probability density function. More details on CSE can be found in [6, 7, 12, 15].

For atmospheric- $p$  situation, the EOS is only mildly non-linear, but, as already mentioned, for real fluids the EOS is strongly non-linear. This means that the thermodynamic variables are strongly correlated which would invalidate Eq. (2.1). One of the manifestation of this correlation would be to find large variances for  $T|\zeta$ ,  $\rho|\zeta$ , or  $Y_i|\zeta$ .

## 3. Overview of the DNS Database

The DNS database developed by Bellan [2] was used as the basis for developing a PDF model. The database, described in detail in [2], represents mixing and turbulent combustion in a high- $p$ , temporally-evolving three-dimensional mixing layer and all scales overwhelmingly responsible for the dissipation have been resolved. The database epitomizes a canonical turbulent reactive flow and thus provides a simple and general configuration to investigate the fundamental physics of the problem.

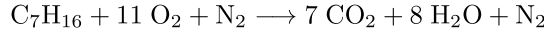
The configuration consists of a fuel ( $C_7H_{16}$ ) and air stream both of which may or may not be slightly vitiated with products of combustion of various compositions; the initial

TABLE 1. Simulation details and resolution.

| Run       | $Re_0$ | $p_0$ (atm) | $N_x \times N_y \times N_z$ | fuel stream<br>( $C_7H_{16}, CO_2, H_2O$ ) | oxidizer stream<br>( $O_2, N_2, CO_2, H_2O$ ) |
|-----------|--------|-------------|-----------------------------|--|---|
| R1000p60  | 1000   | 60          | $480 \times 530 \times 288$ | (0.955, 0.035, 0.001)                      | (0.20, 0.755, 0.035, 0.001)                   |
| R1000p80  | 1000   | 80          | $584 \times 630 \times 344$ | (0.955, 0.035, 0.001)                      | (0.20, 0.755, 0.035, 0.001)                   |
| R1000p60a | 1000   | 60          | $480 \times 530 \times 288$ | (0.955, 0.035, 0.001)                      | (0.245, 0.755, 0.0, 0.0)                      |
| R2000p60  | 2000   | 60          | $768 \times 804 \times 460$ | (0.955, 0.035, 0.001)                      | (0.20, 0.755, 0.035, 0.001)                   |

Reynolds number and free-stream  $p$  are simulation specific. Table 1 lists the simulation parameters. The DNS code solves the compressible conservation equations coupled to the Peng-Robinson (PR) equation of state; for improved accuracy in the high- $p$  regime of PR, a volume shift is implemented, see [8]. A full matrix of the mass-diffusion coefficients and thermal diffusion factors defined in *Masi et al. 2013* and summarized in [2] (see appendix) is used to obtain the solution.

The chemical kinetics are modeled using a single-step reaction mechanism for the oxidation of heptane:



where the reaction rate is

$$\dot{\omega} = AT^n \frac{\rho^2}{m_{C_7H_{16}} m_{O_2}} Y_{C_7H_{16}} Y_{O_2} e^{\frac{-E_a}{R_u T}} \quad (3.1)$$

and the choice of the parameters is inspired by the chemical mechanism described in [9]; the pre- and exponential coefficients are slightly modified [27] to avoid abrupt ignition  $A = 9.6 \times 10^6 \text{ (cm}^3/\text{mol)s}^{-1}$ ,  $E_a = 30 \text{ kcal/mol}$ , and  $n = 0$ . Additionally,  $R_u = 1.98588 \times 10^{-3} \text{ kcal/(K mol)}^{-1}$ .

## 4. Results

### 4.1. The CSE method

#### 4.1.1. Assessing the PDF in high- $p$ combustion

An assessment of the PDF can be made by comparing the unconditional source-term estimation obtained from CSE with the exact values from the DNS. The rationale is that a good source-term estimation is indicative of a correct estimation of the distribution function as the conditional term is here extracted from the DNS. To ensure a sufficient sample, conditional averages and probability density functions are computed in the homogeneous planes ( $x_1, x_3$ ) of the simulation. For this reason, the average (denoted as  $\langle \cdot \rangle$ ) is used in lieu of the filtered values. The approach used to assess the PDF is summarized in Figure 1.

The average of  $\dot{\omega}$  on a plane specified by the  $x_2$  value is taken to determine its planar average  $\langle \dot{\omega} \rangle$ . The exact PDF of  $\zeta$ , as well as the conditional averages  $\langle T | \zeta \rangle$ ,  $\langle \rho | \zeta \rangle$ , and  $\langle Y_i | \zeta \rangle$  are computed using all points on the same  $x_2$  plane. Unless explicitly specified,

the mixture fraction is defined as:

$$\zeta = \frac{vY_{C7H16} - Y_{O2} + Y_{O2,U}}{vY_{C7H16,L} + Y_{O2,U}}, \quad (4.1)$$

where  $v$  is the stoichiometric mass ratio. For all conditional variables, we use 100 discrete bins in the  $\zeta$ -space.

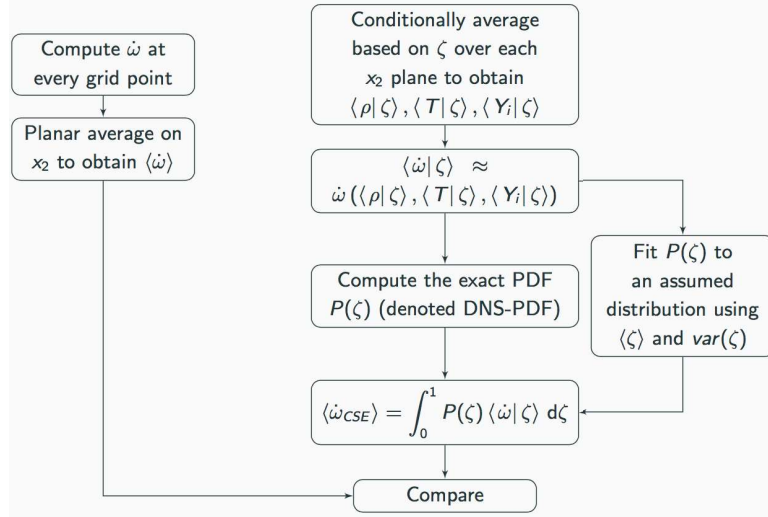
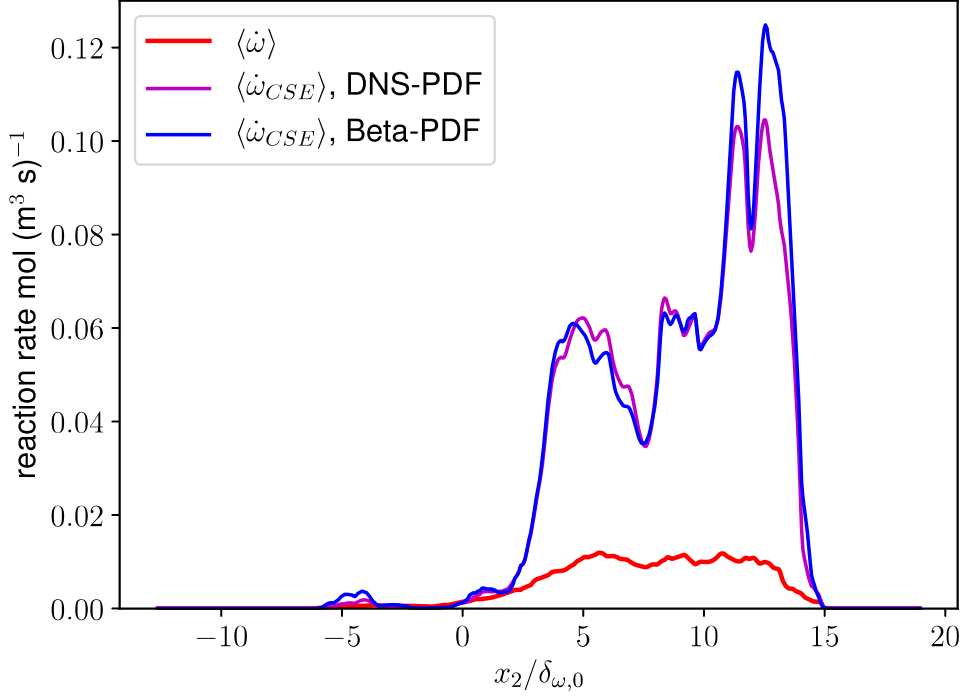


FIGURE 1. Algorithm to evaluate the probability density function.

The approximation of  $\langle \dot{\omega} \rangle$  using the exact PDF of  $\zeta$  can then be computed with Equations (2.1) and (2.2). This approximation is denoted DNS-PDF, and corresponds to the best outcome of CSE if the PDF modeling is assumed to be perfect. To perform CSE with a Beta PDF distribution,  $\langle \zeta \rangle$  and  $var(\zeta)$  are computed in the  $x_2$  plane, and the two moments are used to compute the Beta distribution. For other distributions, different quantities may need to be computed. This is the standard method for CSE, except that with the transported quantities in LES, an inversion process must be performed to determine  $\langle T | \zeta \rangle$ ,  $\langle \rho | \zeta \rangle$ , and  $\langle Y_i | \zeta \rangle$  (equivalently for the filtered conditional values in LES). With DNS data, these conditional averages can be computed without an inversion process. To reduce computation time, the conditional averages are often computed over the entire domain, rather than per plane. This approximation is justified by the assumption that the conditional variance is small and the conditional variables do not vary significantly at various spatial locations.

Figure 2 shows the calculation of the reaction rate as described above. It is evident that even with a perfect description of  $P(\zeta)$ , the CSE method results in a significant overestimate of  $\langle \dot{\omega} \rangle$ . The reason for the failure of CSE in this case can be easily explained by Figure 3, which highlights the joint PDF of  $\zeta$  and  $T$ . Since  $var(T | \zeta)$  is large and Equation (3.1) is very non-linear in  $T$ , the underlying assumption of CSE in Equation (2.1) is not valid.

A more accurate model for the PDF of  $\zeta$  will not result in a more accurate estimation of  $\langle \dot{\omega} \rangle$ , due to the shortcomings of the CSE assumptions. In many other flows, particularly at low- $p$  conditions, the underlying assumptions of CSE are valid. In those cases, the accuracy of the PDF model largely determines the accuracy of the CSE method. It is therefore useful to obtain a more accurate model of the  $\zeta$  PDF.

FIGURE 2.  $\langle \dot{\omega} \rangle$  in each  $x_2$  plane, Re1000p60 case.

#### 4.1.2. Mixture Fraction Effect on Distribution Function

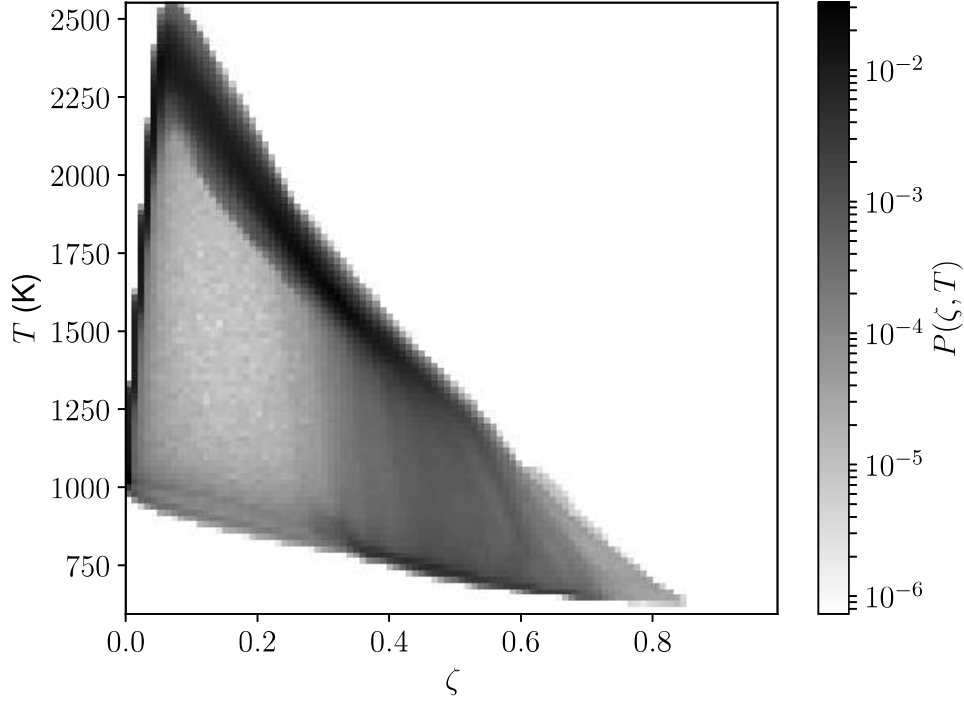
The definition of the mixture fraction may have an effect on the accuracy of the PDF model. If one definition has a PDF distribution that is closer to the Beta distribution or another known distribution, then it may result in a more accurate PDF estimation. For this reason, two common definitions of the mixture fraction are investigated here. The first is the classical mixture fraction definition defined in Eq. (4.1). The following mixture fraction definition, commonly used, is attributed to Bilger [11]:

$$\zeta = \frac{Z_C/(7m_C) + Z_H/(16m_H) + 2(Y_{O_2,U} - Z_O)/(v_{O_2}m_{O_2})}{Z_{C,U}/(7m_C) + Z_{H,U}/(16m_H) + 2Y_{O_2,L}/(v_{O_2}m_{O_2})}. \quad (4.2)$$

Figure 4 compares the PDFs obtained from these two definitions. The difference in terms of PDF shape is minimal, and therefore does not have a large effect on the accuracy of the modeled PDF. For all other results in this report, the mixture fraction is computed with Equation (4.1). It should be noted that the single-step chemistry limits the degrees of freedom of the problem, making both mixture fraction definitions similar. Therefore, an extended investigation of the mixture fraction definition effects should be conducted on DNS with more complex chemical kinetics.

#### 4.1.3. Convolution-Beta PDF

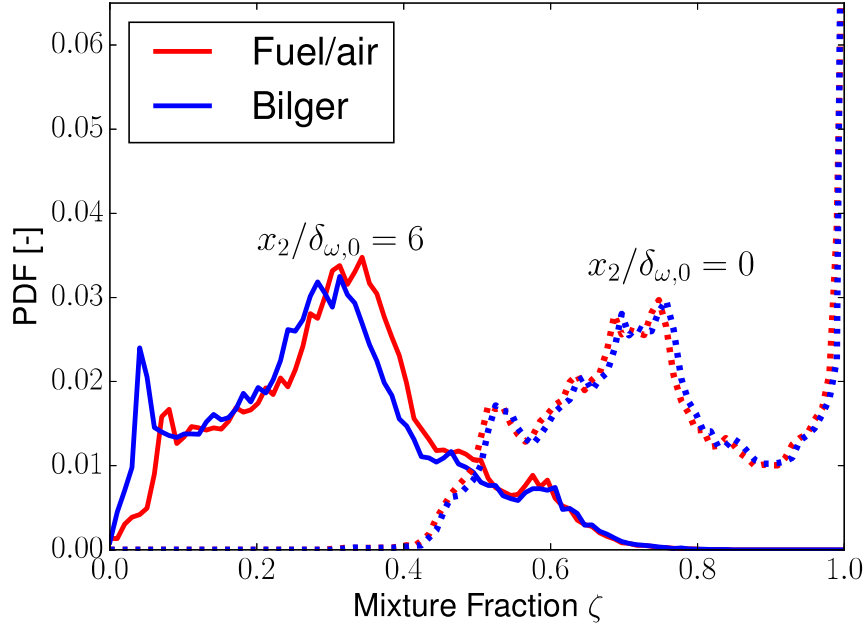
It is evident from the observation of multiple local maximas in Equation 4 that the PDF of  $\zeta$  cannot be fully described by a two-moment distribution such as the Beta distribution. For this reason, higher-order PDFs can be used if a precise description of  $P(\zeta)$  is

FIGURE 3. 2D histogram of  $P(\zeta, T)$ , Re1000p60 case

desired. However, the challenges lie in modeling the unclosed terms of the higher-order moment transport equation (e.g. skewness or kurtosis of the mixture fraction), as a result, these approaches have not been investigated. Instead, a model taking advantage of the fact that the mixture fraction can be described by PDFs of  $Y_{C_7H_{16}}$  and  $Y_{O_2}$  is proposed. One Beta PDF is fit to the mean and variance of  $Y_{C_7H_{16}}$ , and another Beta PDF is fit to the mean and variance of  $Y_{O_2}$ . Using Equation (4.1) and the mathematical properties of distribution functions, a PDF for  $\zeta$  can be obtained which is a convolution of  $P_{Y_{O_2}}$  and  $P_{Y_{C_7H_{16}}}$ :

$$P(\zeta = z) = \int_{-\infty}^{\infty} P_{Y_{O_2}}(y) P_{Y_{C_7H_{16}}} \left( \frac{y + z(vY_{C_7H_{16},L} + Y_{O_2,U}) - Y_{O_2,U}}{v} \right) dy \quad (4.3)$$

Figure 5 compares the fit of this Convolution-Beta PDF to the fit of the Beta-PDF. While the Convolution-Beta model is able to generate two local maximas, it has similar or worse accuracy for source-term estimation compared to the Beta PDF. This is likely due to the fact that there is an error in the fit of both  $P_{Y_{O_2}}$  and  $P_{Y_{C_7H_{16}}}$ . If either of the fits is inaccurate, the resulting fit for the PDF of  $\zeta$  is also inaccurate. For this reason, the Beta PDF is preferred over the Convolution-Beta PDF. Since the Beta PDF has been extensively verified for use in CSE, it would not be advisable to change to another PDF model without clear evidence that it gives better accuracy. For this reason, other double-moment PDFs such as the Gamma PDF are not considered here.

FIGURE 4. Comparison of PDFs obtained with different  $\zeta$  definitions, Re1000p60 case.

#### 4.2. The DCSE method

It is apparent from Figure 2 that CSE does not approximate  $\langle \dot{\omega} \rangle$  accurately. The reason for this is that the variance of the conditional variables in Equation (2.1) is too large in high- $p$  combustion. This is primarily due to the high non-linearity of the state equation, as seen in Figure 3. Since the dependence of  $\dot{\omega}$  on temperature is highly non-linear, using  $\langle T | \zeta \rangle$  in this case results in a large error. For this reason, a Doubly-Conditioned Source-term Estimation (DCSE) is proposed.

By conditioning on  $\zeta$  and  $\phi$  (where  $\phi$  is the second conditioning variable), the conditional variance may be further reduced. This method is essentially the same as CSE, except that  $T$ ,  $\rho$ , and  $Y_\alpha$  are conditioned on two variables instead of one. If  $\phi$  is the second conditioning variable, then Equation (2.1) and Equation (2.2) become:

$$\langle \dot{\omega} | \zeta, \phi \rangle \approx \dot{\omega}(\langle \rho | \zeta, \phi \rangle, \langle T | \zeta, \phi \rangle, \langle Y_i | \zeta, \phi \rangle) \quad (4.4)$$

$$\langle \dot{\omega}_{DCSE} \rangle = \int_{-\infty}^{\infty} \int_0^1 P(\phi | \zeta) P(\zeta) \langle \dot{\omega} | \zeta, \phi \rangle d\zeta d\phi \quad (4.5)$$

Typically in DCSE a progress variable [15] or scalar dissipation [3] is used as  $\phi$ . The judicious choice for the second conditioning variable is that it should be very weakly correlated to the first conditioning variable; otherwise there is not much expectation of progress. For this judicious choice, it can be assumed that  $P(\zeta)P(\phi | \zeta) \approx P(\zeta)P(\phi)$ —a very convenient simplification.

In high- $p$  combustion, using a thermo-physical property as  $\phi$  makes sense, since it is the variance of temperature that is responsible for the largest error. It has been suggested in the past to doubly condition on temperature in CMC [12, 13]. For these rea-



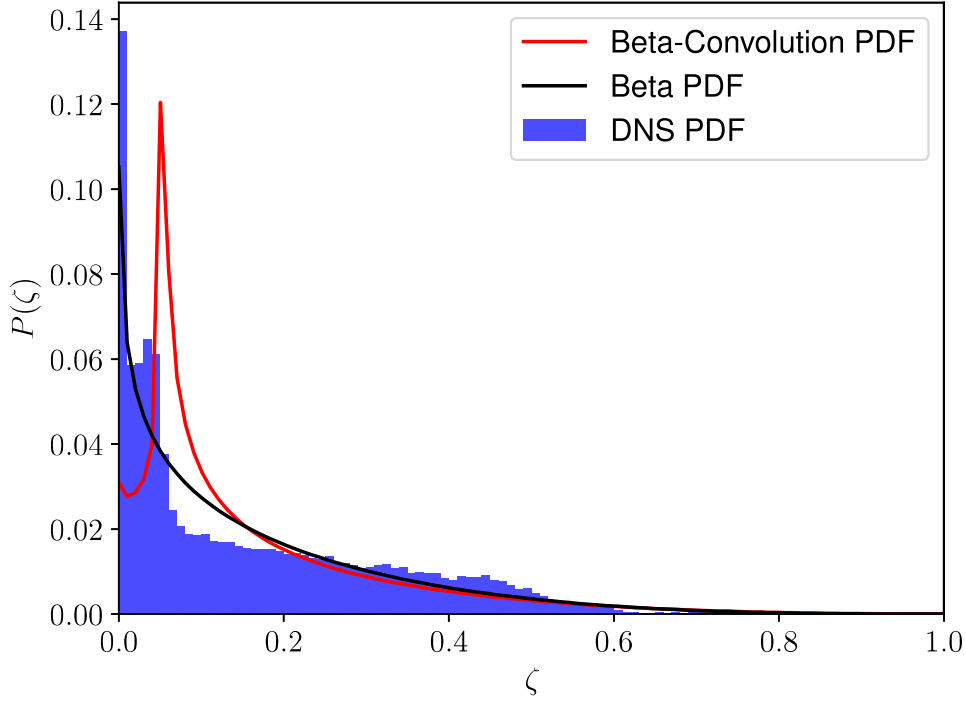


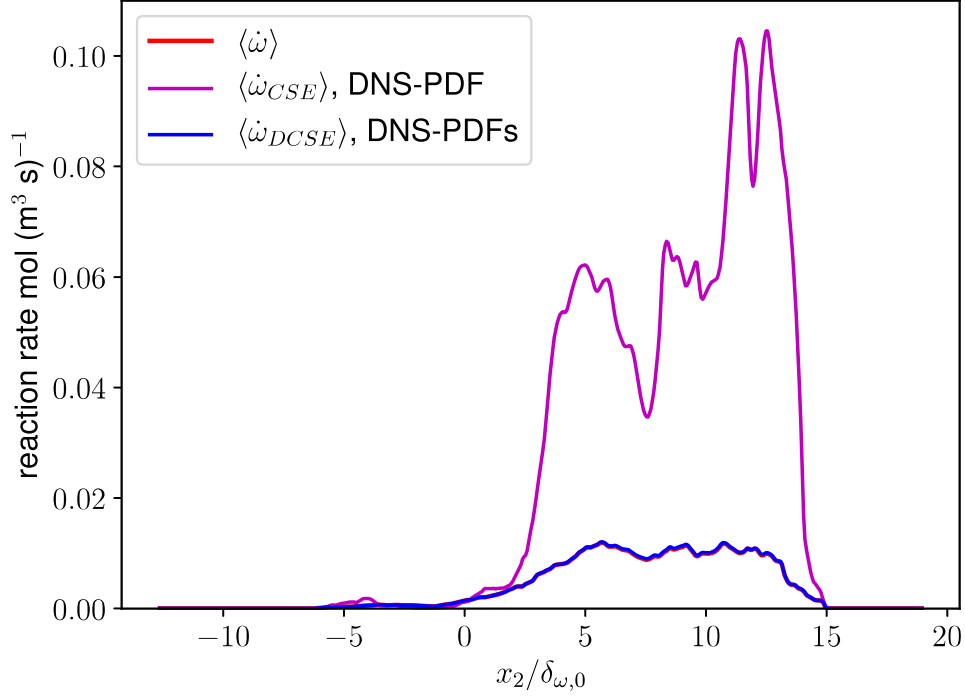
FIGURE 5. Comparison of PDF models, Re1000p60 case.

sons,  $T$  has been used as  $\phi$  for the analysis in this report. As  $T$  is the most important thermodynamic variable for combustion, therefore it represents the most logical variable to reduce the conditional variance resulting from the thermodynamic non-linearities in high- $p$  combustion.

Figure 6 compares the theoretical accuracy of DCSE and CSE methods assuming that the PDF modeling is perfect. It is evident that DCSE is far more accurate than CSE. This is not too surprising since the double conditioning greatly reduces the variance about the conditional mean. Using a Beta distribution instead of the exact PDF results in a slightly increased error but remains significantly better than a single conditioning of the PDF.

In order to use this DCSE method in LES, a PDF distribution must be chosen for  $T$ . Since  $T$  is bounded between the temperature in the unmixed region and the adiabatic flame temperature, these values can be used as a maximum and a minimum in order to normalize  $T$ . The temperature of the unmixed region is well defined as an initial condition, but the adiabatic flame temperature must be computed based on the stoichiometric chemistry. As a starting point, the Beta-PDF has been used to model  $P(T|\zeta)$ . Since it may be more realistic to transport  $var(\rho)$  instead of  $var(T)$ , an extensive study of which PDF model is best for fitting  $P(T|\zeta)$  was not done. The results from DCSE using Beta-PDFs to model  $P(\zeta)$  and  $P(T|\zeta)$  are shown in Figure 7.

In order to validate the DCSE method presented above, CSE and DCSE were applied to all of the DNS cases. The results are shown in Figure 8. In every case, the DCSE method gives a better approximation of  $\langle \dot{\omega} \rangle$  than CSE does. In order to quantify the

FIGURE 6. Comparison of CSE and DCSE to  $\langle \dot{\omega} \rangle$  per  $x_2$  section, Re1000p60 case.TABLE 2. Comparison of methods by error metric, normalized to  $\langle \dot{\omega}_{err} \rangle$  CSE, DNS-PDF

|   | R1000p60 | R1000p60a | R2000p60 | R1000p80 |
|---|----------|-----------|----------|----------|
| CSE, DNS-PDF  | 1        | 1         | 1        | 1        |
| CSE, Beta-PDF   | 1.22     | 0.97      | 1.17     | 0.99     |
| DCSE, DNS-PDFs  | 5.70e-06 | 6.05e-05  | 2.28e-06 | 5.39e-05 |
| DCSE, Beta-PDF for $\zeta$ , Normal-PDF for $T \zeta$ | 0.20     | 0.16      | 0.33     | 0.11     |

accuracy of each method, an error metric has been computed. The definition of this metric is:

$$\langle \dot{\omega}_{err} \rangle = \frac{1}{N_2} \sum_{i=0}^{N_2} (\langle \dot{\omega}_{calc} \rangle - \langle \dot{\omega} \rangle)^2 \quad (4.6)$$

Where  $\langle \dot{\omega}_{calc} \rangle$  is the method used to approximate  $\langle \dot{\omega} \rangle$ , and  $N_2$  is the number of planes in  $x_2$ . The results computed using this metric are shown in Table 2.

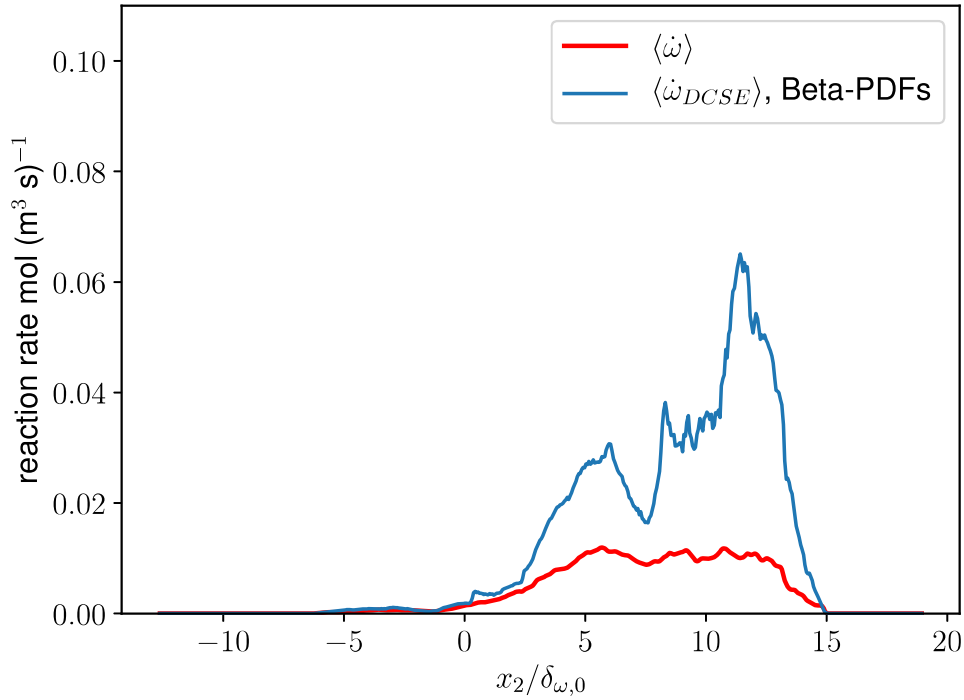


FIGURE 7. Comparison of DCSE with Beta-PDFs to  $\bar{\omega}$  in  $x_2$  specified planes, Re1000p60 case.

## 5. Summary and Conclusions

A unique DNS database of high-pressure turbulent combustion is used to investigate the optimal characterization of the probability density function of the mixture fraction. The developed PDF is then used to compute the average chemical source-terms. It is shown that a conditioning based on the mixture fraction alone is insufficient to account for the combined non-linearity of the chemical source term, non-linear transport and non-linear equation of state. Furthermore, a higher-moment distribution function showed marginal benefit (despite an increase in complexity) in terms of source-term estimation. In other words, compositional information alone is insufficient to fully characterize the chemical source terms in high-p combustion. At these conditions, the thermodynamic effects play a significant role in the chemical kinetics; thus, they must be considered. Given the strongly non-linear coupling between the state variables, as defined by the Peng-Robinson state equation, a doubly-conditioned PDF was investigated. A Doubly-conditioned Chemical Source-term Estimation (DCSE) is proposed to improve the source term modeling. Conditioning the variables on temperature and mixture fraction significantly reduces the variance in conditional space which results in very accurate source-term estimations.

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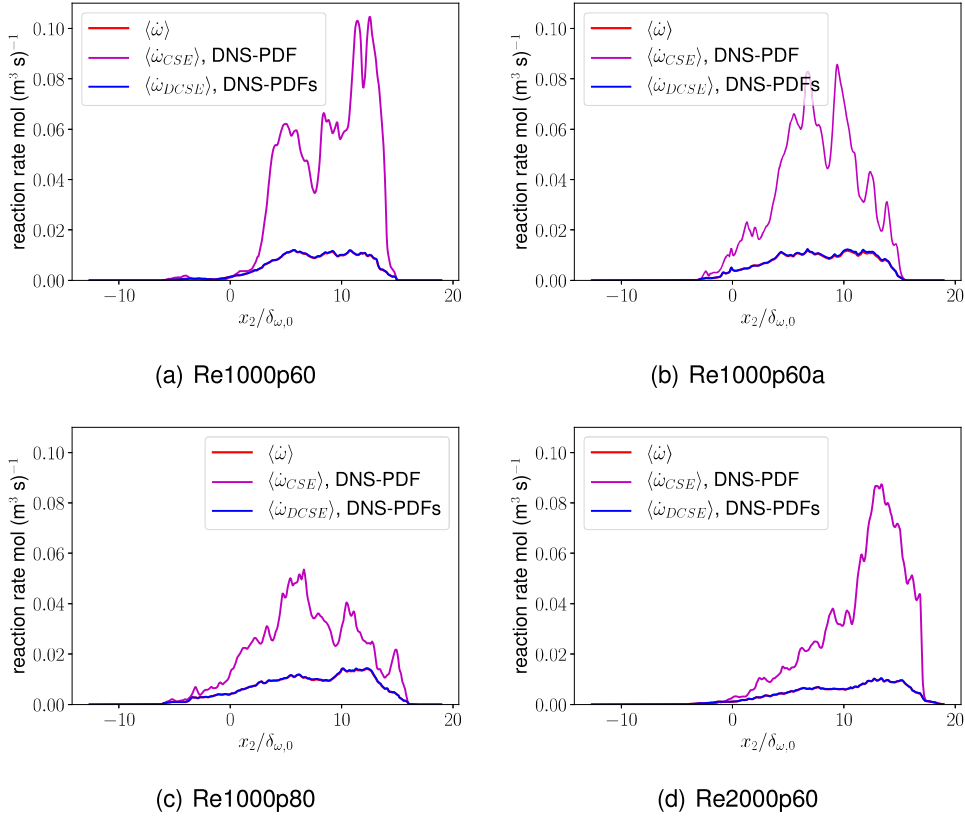


FIGURE 8. Comparison of DCSE and CSE methods, all cases.

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